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MODTRAN: A MODERATE RESOLUTION MODEL FOR LOWTRAN

A. Berk, L. S. Bernstein, and D. C. Robertson
Spectral Sciences, Inc.
111 S. Bedford Street
Burlington, MA 01803-5128

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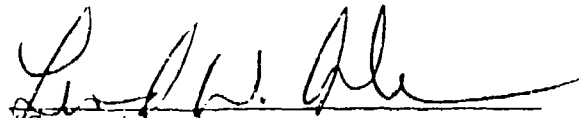
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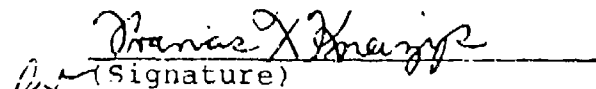
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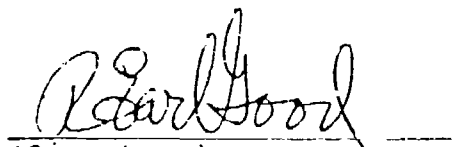
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<p>This interim technical report describes a new band model formulation for the LOWTRAN 6 atmospheric transmittance/radiation computer code. Band model parameters for H_2O, CO_2, O_3, N_2O, CO, CH_4, O_2, and N_2 were calculated using the 1986 HITRAN line atlas. They were calculated for $1/cm$ bins from $0 - 17,900/cm^{-1}$ and at five temperatures from 200 to 300K. This transmittance model and associated subroutines have been integrated into LOWTRAN 6. The spectral resolution of this new option is better than $5/cm$ (FWHM). A preliminary version of the code has been delivered to AFGL for testing. Validation against FASCOD2 calculations will be the emphasis for the remainder of this effort.</p>					
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1.0 INTRODUCTION

This interim technical report describes work done in year one (12 May 1986 - 11 May 1987) of a program (Contract No. F19628-86-C-0079) to increase the spectral resolution of LOWTRAN 6⁽¹⁾ by developing a radiative transfer model and attendant computer subroutines for molecular absorption effects. Specifically, the goals for this effort are to:

- develop algorithms providing at least 3 cm^{-1} resolution (FWHM - full width at half maximum),
- model molecular absorption of atmospheric molecules as a function of temperature and broadening density from 0 to $17,900\text{ cm}^{-1}$,
- treat the following atmospheric molecules: water vapor, ozone, carbon dioxide, methane, nitrous oxide, carbon monoxide, molecular nitrogen and oxygen, and
- integrate the new algorithms and subroutines into LOWTRAN 6.

The upper limit of the spectral range, $17,900\text{ cm}^{-1}$, is determined by the HITRAN line atlas for atmospheric molecules.⁽²⁾

1. F. X. Kneizys, E. P. Shettle, W. O. Gallery, J. H. Chetwynd, Jr., L. W. Abreu, J. E. A. Selby, S. A. Clough and R. W. Fenn, "Atmospheric Transmittance/Radiance: Computer Code LOWTRAN 6," AFGL-TR-83-0187, Air Force Geophysics Laboratory, Hanscom AFB, MA 01731, (August 1983). ADA137786
2. R. A. McClatchey, W. S. Benedict, S. A. Clough, D. E. Burch, R. F. Calfee, K. Fox, L. S. Rothman, and J. S. Garing, "AFCRL Atmospheric Absorption line Parameters Compilations," AFCRL-TR-73-0096, Air Force Geophysics Laboratory, Hanscom AFB, MA 01731 (January 1973); L. S. Rothman, Appl. Opt., 20, 791 (1981). AD762904

A substantial fraction of this work has been completed. Molecular transmittance through the atmosphere has been modeled using standard band model techniques.⁽³⁻⁵⁾ In the present approach, the spectral region is partitioned into 1 cm^{-1} bins for each molecule. Within each bin, contributions from lines whose centers are within the bin and from nearby lines centered outside of that bin are modeled separately with their own temperature and pressure dependences; see Figure 1. The absorption due to lines within the bin is calculated by numerically integrating over the Voigt line shape⁽⁵⁾. The Curtis-Godson^(6,7) approximation, which is accurate for the moderate temperature, pressure, and concentration variations found in the earth's atmosphere, is used to replace multilayered paths by an equivalent isotropic one. The transmittance algorithms have been coded and integrated into LOWTRAN 6. Comparisons to "exact" calculations with FASCOD2^(8,9) resulted in a reexamination of and a new definition for the standard line density band model parameter, $1/d$; this new definition lowers the line center absorption by taking the finite bin widths into account. A complete band model tape has been generated for the molecules listed above. A preliminary version of MODTRAN, this moderate resolution LOWTRAN 6, has been delivered to AFGL for evaluation.

3. D. Anding, "Band Model Methods for Computing Atmospheric Slant Path Molecular Absorption," Rpt. No. 7142-12-T, Willow Run Laboratories, Environmental Research Institute of Michigan, Ann Arbor, MI (1967).
4. A. J. LaRocca and R. E. Turner, "Atmospheric Transmittance and Radiance: Methods of Calculation, Rpt. No. 107600-10-T, Environmental Research Institute of Michigan, Ann Arbor, MI (June 1975).
5. W. L. Wolfe and G. J. Zissis, "The Infrared Handbook: Revised Edition," The Infrared Information and Analysis (IRIA) Center, Environmental Research Institute of Michigan, Ann Arbor, MI (1985).
6. A. R. Curtis, Q. J. R. Meteor. Soc., 78, 165 (1952).
7. W. L. Godson, J. Meteor., 12, 123 (1955).
8. S. A. Clough, "Preliminary User Instructions for FASCOD2," Letter, AFGL/OPI, Hanscom AFB, MA 01731 (1 October 1985).
9. H. J. P. Smith, D. J. Dube, M. E. Gardner, S. A. Clough, F. X. Kneizys and L. S. Rothman, "FASCODE - Fast Atmospheric Signature Code (Spectral Transmittance and Radiance)," AFGL-TR-78-G081, Air Force Geophysics Laboratory, Hanscom AFB, MA 01731 (1978). ADA957506

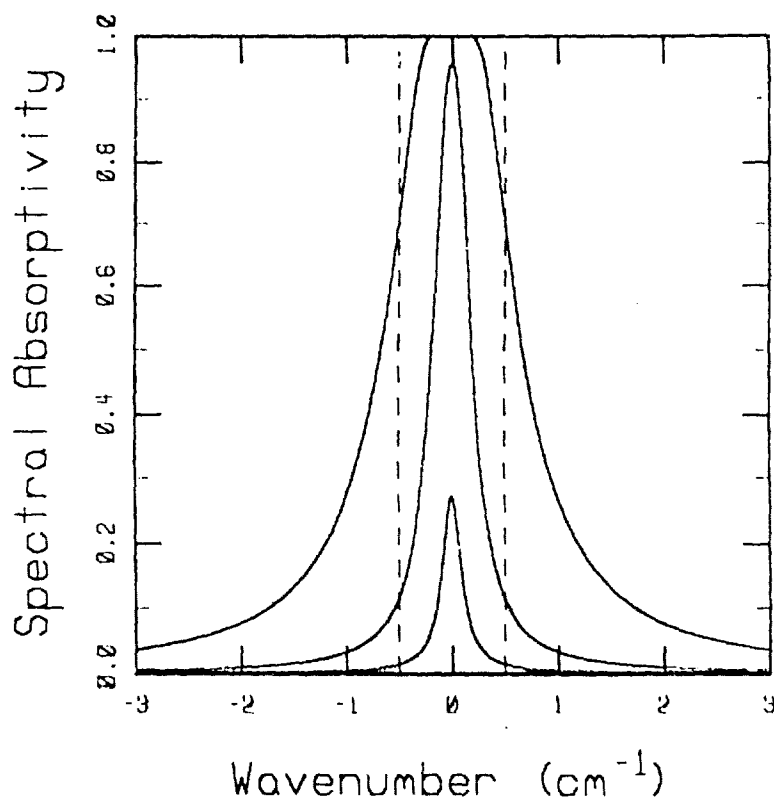


Figure 1. Spectral Absorptivity for Lorentz Line Shapes. Curves Generated for Products of Line Strength and Absorber Amounts Equal to 0.1, 1.0 and 10.0 cm^{-1} . The Halfwidth has been fixed at 0.1 cm^{-1} . In the Band Model Transmittance Formulation, Absorption Due to Lines Whose Centers Are Within a Bin (Between the Dashed Lines) is Modeled Separately from That Due to Line Tail Absorption (Outside the Dashed Lines).

An overview of the MODTRAN code is presented in Section 2. In the subsequent two sections, calculation of the band model parameters and the transmittance formulation are described. Modifications and additions to LOWTRAN 6 are presented in Section 5. In Section 6, MODTRAN output is analyzed for the purpose of validation. Conclusions and future plans are discussed in the final section.

The following indexing convention is used throughout the report:

<u>Symbol</u>	<u>Indexed Quantity</u>
i	spectral bin
m	molecule
n	temperature
σ	species
l	atmospheric layer

The species symbol σ , will refer to either an individual species such as water or ozone, or a mixture of molecules such as the uniformly mixed gases (UMG). The atmospheric layers l are characterized by a fixed temperature, pressure, and molecular constituency. Constants used include:(5)

c	=	speed of light	($2.997924580 \times 10^{10}$ cm sec ⁻¹)
k	=	Boltzmann constant	(1.380662×10^{-16} erg K ⁻¹)
h	=	Planck constant	(6.626176×10^{-27} erg-sec)
N	=	Avogadro constant	(6.022045×10^{23} mole ⁻¹)
T _s	=	Standard temperature used in the HITRAN line atlas	(296 K)
T ₀	=	Standard temperature used in LOWTRAN	(273.15 K)

2.0 THE MODTRAN CODE - AN OVERVIEW

MODTRAN is the name given to the LOWTRAN 6 code affixed with a new moderate resolution radiative transport algorithm. The new subroutines have been written in portable ANSI standard FORTRAN and constructed so that their interfacing with LOWTRAN 6 minimizes coding changes. These additional elements do not interfere with the regular operation of LOWTRAN 6; rather they represent an additional capability for higher spectral resolution. The only modification to the input data sequence is

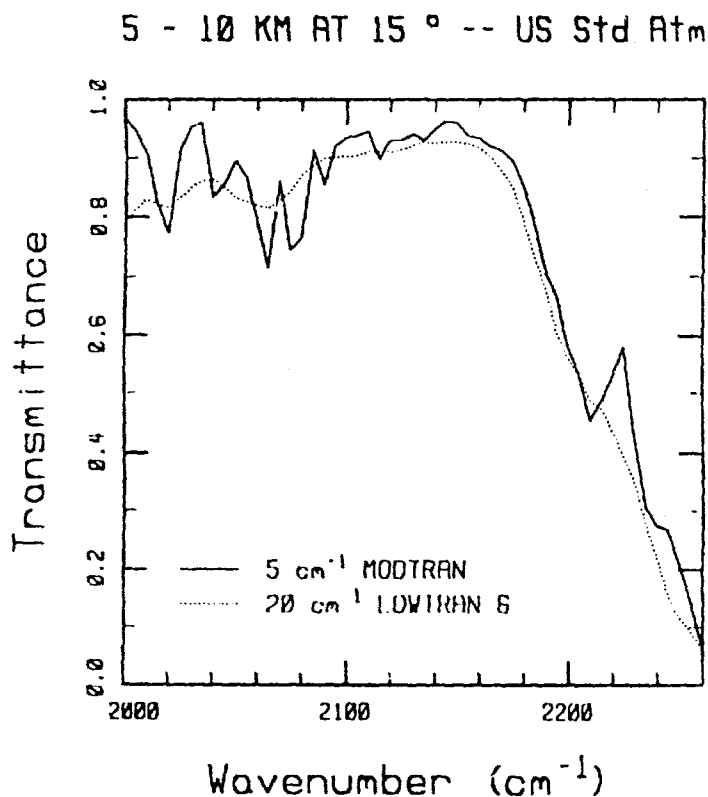


Figure 2. Transmittance Curves for a 15° from Zenith Slant Path from 5 to 10 km Through the US Standard Atmosphere. The Solid Curve was Obtained from MODTRAN by Passing a 5 cm^{-1} FWHM Triangular Slit Over the 1 cm^{-1} Calculation. The Dotted Curve is the Regular LOWTRAN 6 Result also Obtained from MODTRAN (20 cm^{-1} Resolution with DV Set to 5 cm^{-1}).

an additional parameter, JBMOD, which is added to the end of CARD1. The user who is not interested in using the MODTRAN option simply ignores this parameter and prepares his input file in the usual way; the program then functions in its "normal" mode and does not require access to an external data file of band model parameters. When using the band model option (JBMOD = 1), access to this data file is required.

A comparison of MODTRAN and LOWTRAN 6 demonstrates the importance of the higher resolution algorithm. Figure 2 shows transmittance calculated at 5 and 20 cm^{-1} resolution for a low altitude slant path through the US Standard Atmosphere. The 5 cm^{-1} (FWHM) curve results from an internal degradation of 1 cm^{-1} bin transmittances with a triangular slit function, and the 20 cm^{-1} curve is the regular LOWTRAN 6 result as calculated by MODTRAN. If the 5 cm^{-1} calculations were degraded to the 20 cm^{-1} LOWTRAN 6 calculation, the overall agreement would be quite good. However, at higher resolution, large deviations from the lower resolution calculations occur. In particular, the MODTRAN calculation resolves the structure of water lines below 2100 cm^{-1} and the band center of the ν_2 fundamental at 2220 cm^{-1} .

3.0 MOLECULAR BAND MODEL PARAMETERS

The basic assumption of the band model concept^(3,5) is that spectral line positions and strengths are distributed in a way that can be represented by a simple mathematical model. In one approach, the broad frequency continuum of the band models is divided into small bins. The line and tail contributions to each bin, Figure 1, are then parameterized so that the bin transmittance can be calculated when the absorber amounts are known.

We have chosen a bin width of one wavenumber, $\Delta\nu = 1 \text{ cm}^{-1}$. Line data from the HITRAN tape⁽²⁾, the AFGL line atlas, is used to calculate the band model parameters. Since it has data for lines in the frequency range 0 to 17900 cm^{-1} , 17900 bins must be characterized. For each contributing molecule, temperature dependent absorption coefficients and line densities along with a line width parameter are used to parameterize the spectral lines whose centers fall within a given bin; a single temperature dependent absorption coefficient parameter determines the contribution to a bin from the tails of lines centered in nearby bins.

In the next two subsections, the calculation of the molecular band model parameters is described, and the formatting of the data file is discussed in the third subsection. Formulas used to derive the parameters are given, along with a discussion of their dependence on temperature and pressure.

3.1 Line Center Parameters

Each wavenumber bin corresponds to a 1 cm^{-1} interval and contains parameters for molecules with lines in that interval. The molecules for which band model parameters are included are:



The molecular absorption coefficients $(S/d)_0$ ($\text{cm}^{-1} \text{ amagats}^{-1}$, 1 amagat = 1 atm at STP) are calculated at 5 reference temperatures

$$\{T_n\}_{n=1}^5 = \{200 \text{ K}, 225 \text{ K}, 250 \text{ K}, 275 \text{ K}, 300 \text{ K}\} \quad (1)$$

In the band model subroutines, a linear interpolation is used to calculate absorption coefficients at temperatures between 200 and 300 K. For temperatures below 200 and above 300 K, the extreme values, $(S/d)_1$ and $(S/d)_5$, respectively, are used. The molecular absorption band model parameters are calculated from the individual line strengths,

$$(S/d)_n = \frac{1}{\Delta\nu} \sum_j S_j(T_n) \quad (2)$$

Here $S_j(T_n)$ is the integrated line strength at temperature T_n of the j 'th line of molecule m in bin i . The line strength at an arbitrary temperature can be scaled from the HITRAN line strength at its standard temperature, T_s , by

$$S_j(T_n) = \frac{Q_r(T_s)Q_v(T_s)}{Q_r(T_n)Q_v(T_n)} \frac{1}{1 - \exp(-hc\nu_j/kT_n)} \exp\left(-\frac{E_j}{k} \frac{T_n - T_s}{T_n T_s}\right) S_j(T_s) \quad (3)$$

where Q_r and Q_v are the rotational and vibrational partition functions, and E_j is the energy of the lower transition state.

A collision broadened or Lorentz line width parameter $(\gamma_c)_0$ is defined at STP ($T = T_0 = 273.15 \text{ K}$, $P = P_0 = 1013.25 \text{ mbars}$). A single value can be stored because the pressure and temperature dependence of the Lorentz line width is easily modeled.

$$\gamma_c(T,P) = (\gamma_c)_0 \frac{P}{P_0} (T_0/T)^{x_m} \quad (4)$$

where the exponent x_m has been set to 1/2 for all molecules except CO_2 , for which $x_{\text{CO}_2} = 3/4$. The $(\gamma_c)_0$ band model parameter is calculated as a line strength weighted average over the tabulated Lorentz line widths $(\gamma_c)_j(T_s)$ at $P = P_0$, $T = T_s$

$$(\gamma_c)_0 = (T_s/T_0)^{x_m} \left[\sum_j (\gamma_c)_j(T_s) S_j(T_s) \right] / \left[\sum_j S_j(T_s) \right] \quad (5)$$

like the absorption coefficients, the line density band model parameters $(1/d)_n$ (cm) are calculated at the 5 reference temperatures and interpolated when used by the band model subroutines. The line density is defined by

$$(1/d) = \frac{1}{\Delta\nu} \left(\sum_{j=1}^N S_j \right)^2 / \sum_{j=1}^N S_j^2 \quad (6)$$

This definition for the line spacing, which is derived in the appendix, differs from the usual definition involving a sum over the square root of the line strengths^(3,4,10,11).

3.2 Line Tail Parameters

The line tail parameters consist of line contributions from lines located outside of a given bin but within $\pm 25 \text{ cm}^{-1}$. The line tail absorption coefficient band model parameters C_n ($\text{cm}^{-1} \text{ amagat}^{-1}$) are determined by integrating the Lorentz line shape over this interval.

$$C_n = \frac{1}{\pi \Delta\nu} \sum_{k=i-25}^{i+25} (1 - \delta_{ki}) \frac{[(S/d)_n \gamma_c(T_n, P_0)]_k}{(k-i)^2 + 1/4} f[(k-i)\Delta\nu] \quad (7)$$

where the delta function serves to exclude the $k=i$ term from the sum (i.e., the line center contribution). For molecules other than H_2O and CO_2 , tail contributions beyond 25 cm^{-1} from a line center have been assumed to make a negligible contribution to the transmittance and within the 25 cm^{-1} limit a

10. D. C. Robertson, L. S. Bernstein, and R. Haines, "Addition of a 5 cm^{-1} Spectral Resolution Band Model Option to LOWTRAN 5," ARL RR 232 Aerodyne Research, Inc., Billerica, MA (October 1980).
11. D. C. Robertson, L. S. Bernstein, R. Haines, J. Wunderlich, and L. Vega, " 5 cm^{-1} Band Model Option to LOWTRAN 5," Appl. Opt., **20**, 3218 (1981).

form factor, $f[(k-i)\Delta\nu]$, equal to 1 has been assumed. The usual LOWTRAN 6 water continuum consists of the tail contributions beyond 25 cm^{-1} plus extrapolated values of the contribution within 25 cm^{-1} (for smoothness). For CO_2 , the continuum from the FASCOD2^(8,9) has been added to C_n to account for the tail contributions from lines beyond 25 cm^{-1} .

$$C_n \rightarrow C_n + \nu_i \tanh\left(\frac{h\nu_i}{2kT_n}\right) \frac{T_s}{T_n} \hat{C}(\nu_i) \quad (8)$$

Here, $\hat{C}(\nu_i)$ is the frequency interpolated value from FASCOD2's block data /FCO2/. For both H_2O and CO_2 , the value of C_n has also been reduced by an amount equal to the 25 cm^{-1} from line center contribution since this contribution is included already in the continuum data.⁽¹²⁾ The C_n are taken to be proportional to pressure

$$C_n(P) = \frac{P}{P_0} C_n(P_0) \quad (9)$$

3.3 Parameter Data File

Because of the large amount of data, the file for the band model parameters is an external file written in binary format which allows for quicker access during the calculation. Each entry corresponds to a 1 cm^{-1} interval and contains a molecular parameter set. Zeroed data are not stored for molecules contributing no lines to a given interval. Therefore, information which labels the parameter set must also be stored.

The first entry of a parameter set is the bin number, i . From the bin number, the midpoint of the interval is easily calculated

$$\nu_i = i \Delta\nu \quad (10)$$

and all lines whose centers fall in the half opened interval $(\nu_i - \Delta\nu/2, \nu_i + \Delta\nu/2]$ contribute to bin i .

¹² S. A. Clough, personal communication.

A number m between 1 and 8 designates the molecule. Except for N_2 , we follow the convention set by the HITRAN tape⁽²⁾

m	1	2	3	4	5	6	7	8
molecule	H_2O	CO_2	O_3	N_2O	CO	CH_4	O_2	N_2

The next entries in the parameter set are the molecular absorption coefficients $(S/d)_n$ (cm^{-1} amagats⁻¹) calculated at the five reference temperatures. These entries are followed by the STP Lorentz half width, $(\gamma_c)_0$, multiplied by 10^4 and stored as an integer. Line spacing parameters (l_d) for the five reference temperatures complete the line center parameter sets.

Each parameter set for line tails contains information on one or two molecules. These line tail parameter sets use the same format as the line center parameter sets. Again, the first entry is the bin number i and the second entry is the molecule designation m . To recognize that these parameter sets denote line tail contributions, their molecule labels are offset by 8

m	9	10	11	12	13	14	15	16
molecule	H_2O	CO_2	O_3	N_2O	CO	CH_4	O_2	N_2

The continuum parameters, C_n , are stored in place of the $(S/d)_n$. The molecular designation and continuum parameters for a second molecule can be entered in place of the half width and $(l/d)_n$ parameters.

4.0 BAND MODEL TRANSMITTANCE FORMULATION

4.1 Line Center Transmittance

The band model transmittance formulation^(10,11) developed for the 5 cm⁻¹ option to LOWTRAN 5⁽¹³⁾ has been used to create a moderate resolution option for LOWTRAN 6.⁽¹⁾ The expression used to calculate molecular transmittance due to line centers is based on a statistical model for a finite number of lines in a spectral interval, and is given by

$$\tau = (1 - \langle W_{sl} \rangle / \Delta\nu)^{\langle n \rangle} \quad (11)$$

where τ is the transmittance, $\langle W_{sl} \rangle$ is the path averaged single line equivalent width for the line strength distribution in a spectral interval, and $\langle n \rangle$ is the path averaged effective number of lines in the bin

$$\langle n \rangle = \Delta\nu \langle 1/d \rangle \quad (12)$$

$\langle 1/d \rangle$ is the path averaged line spacing.

For large $\langle n \rangle$ [(S/d) and $\Delta\nu$ fixed], the transmittance simplifies to a more recognizable exponential form given by

$$\tau \approx \exp(-\langle W_{sl} \rangle \langle 1/d \rangle) \quad \text{for } \langle n \rangle \text{ large} \quad (13)$$

For the molecular species and relatively low temperatures encountered in the earth's atmosphere, the average number of lines in a bin is usually small so that the power law transmittance approximation is preferred.

There are many approximations available for calculating the equivalent width of a Voigt line shape; different ones are valid for different

13. F. X. Kneizys, E. P. Shettle, W. O. Gallery, J. H. Chetwynd, Jr., L. W. Abreu, J. E. A. Selby, R. W. Fenn, and R. A. McClatchey, "Atmospheric Transmittance/Radiance: Computer Code LOWTRAN 5," AFGL-TR 80-0067, Air Force Geophysics Laboratory, Hanscom AFB, MA 01731 (February 1980). ADA088215

regimes, Doppler or collision broadening, weak line or strong line, etc.

However, no single approximation is adequate for the range of pressures and optical path lengths encountered in atmospheric transmission calculations. Rather than incorporating different approximations, we directly evaluate the exact expression for the equivalent width of a single line with a Voigt line shape; $\langle W_{sl} \rangle$ is given by

$$1 - \frac{\langle W_{sl} \rangle}{\Delta \nu} = \frac{1}{X_m} \int_0^{X_m} \exp \left\{ -[Su/d] \sqrt{\ln 2/\pi} F(X,Y) / \langle \gamma_d/d \rangle \right\} dX \quad (14a)$$

$$F(X,Y) = \frac{Y}{\pi} \int_{-\infty}^{\infty} \frac{\exp(-T^2) dT}{Y^2 + (X-T)^2} \quad (14b)$$

$$X_m = \frac{1}{2} \sqrt{\ln 2} \langle n \rangle / \langle \gamma_d/d \rangle \quad (14c)$$

$$Y = \sqrt{\ln 2} \langle \gamma_c/d \rangle / \langle \gamma_d/d \rangle \quad (14d)$$

where $F(X,Y)$ is the Voigt line shape function and $\langle \gamma_d/d \rangle$ and $\langle \gamma_c/d \rangle$ are path averaged Doppler and collision broadened line shape parameters respectively. The factor of 1/2 in Eq. (14c) corresponds to the half width of the spectral interval.

4.1.1 Curtis Godson Approximation

Path averages are calculated with the Curtis Godson approximation. (6,7,14) This approximation replaces an inhomogeneous path with a homogeneous one by using average values for the various band model

14. C. B. Ludwig, W. Malkmus, J. E. Reardon and J. A. L. Thomson, "Handbook of Infrared Radiation from Combustion Gases," NASA Report SP 3080 (1980).

parameters. The Curtis Godson approximation is very good for paths where the temperature or species gradient is not particularly steep. This is certainly the case for atmospheric paths where the temperature variations for arbitrary paths fall within the range of 200 to 300 K. The total optical depth is a sum over contributions from the individual layers and is given by

$$[Su/d] = \sum_k (S/d)_k (\Delta u)_k \quad (15)$$

where $(\Delta u)_k$ is the incremental absorber amount from layer k and $(S/d)_k$ is the absorption coefficient band model parameter at the temperature dictated by the layer index, k . Note, frequency and species indices are implicitly assumed for this and the subsequent equations.

The total optical depth is used as the weighting function in calculating the path averages

$$\langle 1/d \rangle = \frac{1}{[Su/d]} \sum_k (1/d)_k (S/d)_k (\Delta u)_k \quad (16)$$

$$\langle \gamma_c/d \rangle = \frac{1}{[Su/d]} \sum_k (\gamma_c)_k (1/d)_k (S/d)_k (\Delta u)_k \quad (17)$$

$$\langle \gamma_d/d \rangle = \frac{1}{[Su/d]} \sum_k (\gamma_d)_k (1/d)_k (S/d)_k (\Delta u)_k \quad (18)$$

These band model parameters were defined in the previous section, and $(\gamma_d)_k$ is the usual Doppler width (cm^{-1})

$$\begin{aligned} (\gamma_d)_k &= (\gamma_d)_{i,\sigma}(T) \\ &= \frac{v_i}{c} \sqrt{2(\ln 2)NkT/M} \end{aligned} \quad (19)$$

with M equal to the molecular mass (g/mole) and σ the species index.

4.1.2 Uniformly Mixed Gases

Thus far, we have implicitly assumed that the species σ in LOWTRAN are simply molecules m . In actuality, LOWTRAN 6 assumes a uniformly mixed gas (UMG) with the molecules CO_2 , N_2O , CO , CH_4 , and O_2 combined according to atmospheric mixing ratios, χ_m . (15)

molecule:	CO_2	N_2O	CO	CH_4	O_2
χ_m	3.3×10^{-4}	2.8×10^{-7}	7.5×10^{-8}	1.6×10^{-6}	2.095×10^{-1}

Band model parameters for the nonuniformly mixed gases, H_2O and O_3 , were calculated individually according to the equations from the subsection 3.1. For the UMG, the individual band model parameters were combined according to their ratios

$$(S/d)_n^{\text{UMG}} = \sum_m \chi_m (S/d)_{n,m} \quad (20)$$

$$(1/d)_n^{\text{UMG}} = [(S/d)_n^{\text{UMG}}]^2 / \sum_m [\chi_m^2 (S/d)_{n,m}^2 / (1/d)_{n,m}] \quad (21)$$

$$(\gamma_c)_o^{\text{UMG}} = \frac{1}{(S/d)_n^{\text{UMG}}} \sum_m \chi_m (\gamma_c)_{o,m} (S/d)_{o,m} \quad (22)$$

$$(\gamma_d)^{\text{UMG}} = \frac{v_i}{c} \sqrt{2(\ln 2) N k T / M^{\text{UMG}}} \quad (23)$$

with

$$M^{\text{UMG}} = \frac{1}{(S/d)_n^{\text{UMG}}} \sum_m \chi_m M_m (S/d)_{o,m} \quad (24)$$

15. R. A. McClatchey, R. W. Fenn, J. E. A. Selby, F. E. Volz, and J. S. Garing. "Optical Properties of the Atmosphere," 3rd ed., AFGL 72 0497, Air Force Cambridge Research Laboratories, Hanscom AFB, MA 10731 (24 August 1972). AD753075

Here, the subscript m indexes molecules (skipping H₂O, O₃ and N₂ in the sum), a subscript zero has been added to (S/d) for the standard temperature interpolated absorption coefficient, and the superscript UMG labels the uniformly mixed gases species. Again, we have suppressed usage of a bin index.

4.2 Line Wing Absorption

The power law transmittance, eq. (11), takes into account only lines which originate within a given spectral interval, and, for these lines, only that fraction of the line profile which falls within the interval is included in the computation of the equivalent width. This approximation is reasonable in the strongly absorbing region of a band; however, because the absorptivity is expressed in terms of the local line strength distribution, it becomes a poor approximation in regions where the tail contributions from nearby lines dominate the contributions from weak or nonexistent lines within a given interval (bin). This typically occurs in the center and far wings of a band (i.e., past the band head), and also in spectral intervals containing no lines which are in the vicinity of strong lines. For these situations, the local absorption is dominated by the accumulated tails of the stronger lines originating outside the interval. The effect of line wing absorption is included in the transmittance by adjoining an exponential term

$$\tau = (1 - \langle W_{sl} \rangle / \Delta \nu)^{\langle n \rangle} e^{-[Cu]} \quad (25)$$

where [Cu] is the total continuum optical depth

$$[Cu] = \sum_l (C)_l (\Delta u)_l \quad (26)$$

The layer subscript l on C labels both the pressure and temperature.

5.0 INTEGRATION INTO LOWTRAN 6

Integration of the MODTRAN subroutines into LOWTRAN 6 has been accomplished with minimal changes to the original code. The interface between the regular LOWTRAN 6 and the MODTRAN option is made through calls to two subroutines in the LOWTRAN 6 subroutine TRANS. A single call to subroutine BMDATA reads the first necessary wavenumber block of band model parameters and calculates wavenumber independent quantities. For each wavenumber, calls to subroutine BMOD are made once for initialization and then additionally in the loop over atmospheric layers that calculates the molecular transmittance.

5.1 MODTRAN Subroutines

The MODTRAN subroutines are described in this section. In total, these seven subroutines contain less than 750 lines of code.

5.1.1 Subroutine BMDATA

Subroutine BMDATA is called once each calculation by subroutine TRANS. This subroutine reads the binary band model tape header, makes the initial call to subroutine CONDEN, and calculates wavenumber independent quantities for subsequent use by subroutine BMOD.

After reading the file header, BMDATA checks the wavenumber range requested by the user to see if it falls within the range in the file. If the requested interval is totally outside of the band model parameter range, the program stops with an error message. However, if the requested wavenumber interval is only partially outside of the allowed range, the program readjusts the upper and/or lower wavenumbers to the file's values and proceeds with the calculation. The next read statement skips over wavenumber blocks in the file until it reaches the wavenumber block containing V1, the initial wavenumber.

If the option $IRPT = 4$ is used, the next calculation has the same atmospheric and path parameters but a new wavenumber range. In this case, the call to `BMDATA` only rewinds the file and performs the initial reads. The common block `/CARD5/` was added to pass the value of $IRPT$ to `BMDATA`.

When using the `MODTRAN` option, the array `WPATH` contains the incremental absorber amounts for each layer. However, `WPATH` is not calculated by subroutine `PATH` when the path lies completely within one atmospheric layer, so it must be specified in subroutine `BMDATA` for use by subroutine `BMOD`. Finally, several wavenumber independent quantities for each layer are calculated in `BMDATA` and stored in the appropriate arrays for later use by `BMOD`. These are \sqrt{T} , the pressure normalized to one atmosphere (P/P_0), and the temperature indices for interpolation of the band model parameters.

5 1.2 Subroutine `CONDEN`

Subroutine `CONDEN` makes binary file reads of the band model parameter tape. The tape contains information on each molecule separately. To form the UMG parameters, as required by the `LOWTRAN 6` structure, subroutine `CONDEN` also condenses the molecular information

Data is only stored for molecules contributing to a spectral interval; therefore, it is convenient to use recurrence formulas to sum over molecules for defining the UMG band model parameters:

$$(S/d)_n^{(m+1)} = (S/d)_n^{(m)} + \chi_{m+1} (S/d)_{n,m+1} \quad (27)$$

$$(1/d)_n^{(m+1)} = [(S/d)_n^{(m+1)}]^2 / \{ [(S/d)_n^{(m)}]^2 / (1/d)_n^{(m)} + \chi_{m+1}^2 (S/d)_{n,m+1}^2 / (1/d)_{n,m+1} \} \quad (28)$$

$$(\gamma_c)_o^{(m+1)} = \frac{1}{(S/d)_o^{(m+1)}} \{ (\gamma_c)_o^{(m)} (S/d)_o^{(m)} + \chi_{m+1} (\gamma_c)_{o,m+1} (S/d)_{o,m+1} \} \quad (29)$$

$$M^{(m+1)} = \frac{1}{(S/d)_o^{(m+1)}} \{ M^{(m)} (S/d)_o^{(m)} + \chi_{m+1} M_{m+1} (S/d)_{o,m+1} \} \quad (30)$$

where the superscripts denote the level of recurrence, i.e. (m) and (m+1) are the old and new value, respectively, of the UMG band model parameters. Note, these equations are derived from Eqs. (20) through (24).

5.1.3 Subroutine BMOD

Subroutine BMOD calculates the transmittance using the statistical band model described in Section 4. An initialization call is made once every wavenumber from subroutine TRANS, and subsequent calls are made for each layer to calculate the transmittance. On the first call, BMOD calls CONDEN if the next block of band model parameters needs to be read (IW is the counting variable) and then zeros out quantities for the transmittance calculations. On the subsequent call(s), BMOD calculates the total optical depth and transmittance for each species. The continuum contributions due to tails of lines originating outside the 1 cm^{-1} interval are included in the calculation. BMOD returns the transmittance for the molecular species to TRANS. The transmittances are stored in the regular LOWTRAN 6 transmittance array (TX).

The call(s) made by TRANS to BMOD for calculating the transmittance is embedded in a loop over atmospheric layers. When only transmittance is calculated, the DO loop in TRANS consists of one pass. When atmospheric radiation is calculated, the TRANS loop is over all layers, because the radiation depends on the incremental change in transmittance for each layer. The Curtis Godson approximation for the statistical band model also requires the contribution from each layer for transmittance calculations. In keeping with the philosophy of minimizing changes to the basic LOWTRAN 6 program, this layer loop is done in BMOD for transmittance only.

calculations and in TRANS for radiation calculations. Thus, the layer loop in BMOD consists of just one pass when TRANS is looping over all layers and vice versa. Subroutine BMOD determines whether the loop in TRANS is over one layer or all layers and then adjusts its own loop variable accordingly.

The absorber densities (WPATH) calculated in LOWTRAN are converted to the units of cm amagats in BMOD to be consistent with the units of the band model parameters. The absorber density conversion factors from the regular LOWTRAN 6 units to those used in MODTRAN are:

<u>SPECIES</u>	<u>LOWTRAN 6</u>		<u>MODTRAN</u>
H ₂ O	1 g/cm ²	=	1.25 x 10 ³ cm amagat
OMG	1 km	=	1.0 x 10 ⁵ cm amagat
O ₃	1 cm amagat	=	1 cm amagat

where 1 amagat = 1 atm at STP.

The curve of growth used in the statistical model is based on the equivalent width of a single average line in an interval. The equivalent width and line center transmittances are calculated by subroutine EWIDTH using a Voigt line shape to combine the Doppler and Lorentz line shapes. The Curtis Godson approximation is used to calculate the Lorentz half width (S1), Doppler half width (S2) and line density (S3) for the equivalent homogeneous path. The effective number of lines is also calculated.

In addition to the molecular contributions from lines within each 1 cm⁻¹ spectral interval, contributions from tails of lines external to that interval are also calculated. Since these tails have a smooth spectral structure, they form a continuum component, and the simple exponential form is used to calculate the transmittance. These tail contributions and the molecular components are combined (multiplied together) and stored in the matrix TX for subsequent use by subroutine TRANS.

5.1.4 Subroutine CALC

CALC is called by subroutine BMOD to determine the band model parameters for arbitrary temperatures. The tabulated band model parameters are linearly interpolated over temperature for each layer. If the atmospheric temperature is outside of the temperature range of the tabulated parameters, the entry for either the lowest or highest temperature is returned.

5.1.5 Subroutine EWIDTH

EWIDTH is called by subroutine BMOD to calculate the equivalent width of a single average line for the 1 cm^{-1} interval in addition to the line center transmittance. As discussed in Subsection 3.1, the Voigt line shape is numerically integrated over the full interval. When the optical depth at the line center is less than X_{MIN}/π , Beer's law is used. Otherwise EWIDTH compares the relative values of the Doppler and Lorentz half widths and selects the proper formula for the numerical integration.

Several numerical approximations are used in calculating the equivalent width. The Voigt line shape function is the real part of the complex error function⁽¹⁶⁾ and is calculated in subroutine CPF12. The region out to three half widths is calculated by using a linear approximation in the integration interval. From a study of various combinations for the number of integration intervals for each half width (ISTEP) and the number of half widths from the line center (NALF), integrating out to three half widths in six steps was found to represent a reasonable tradeoff between numerical accuracy and execution time. The region beyond three half widths of the line center is calculated using an asymptotic expression.

16. M. Abramowitz and I. A. Stegun, "Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables," NBS Applied Mathematics Series 55 (December 1965).

5.1.6 Subroutine ERFU

ERFU is used by EWIDTH to calculate the error function. A polynomial approximation which is accurate to better than 2.5×10^{-5} is used.⁽¹⁶⁾

5.1.7 Subroutine CPF12

CPF12 is called by EWIDTH to calculate the complex error function⁽¹⁷⁾ and its first derivative. The real part is the Voigt line shape function, and the first derivative is used to approximate its frequency dependence when performing the integration in EWIDTH. The complex error function subroutine, which was developed by J. Humlicek,⁽¹⁸⁾ is based on a 12'th order Hermite polynomial approximation. An 8'th order approximation was investigated, but the results were not sufficiently accurate.⁽¹⁰⁾

5 2 Modifications to LOWTRAN 6

An attempt has been made to minimize modifications to LOWTRAN 6. As mentioned in the beginning of this section, the switch JBMOD has been added to /CARD1/. Only if JBMOD equals 1 are any changes initiated.

A few routines have required minor modifications. In the MAIN, JBMOD is read and the band model parameter file is opened. Also, MAIN has been modified so that a divide by zero error does not result when ALAM1 is determined at a frequency of 0 cm^{-1} . The molecular column density in STDMDL and the pressure for each atmospheric layer in GEO are now stored in common blocks for use by the MODTRAN subroutines.

The straightforward application of the band model transmittance formulation to the single scattering model in LOWTRAN 6 would require doubling of all layer dimensions and storage of too many path data points.

17. R. M. Goody, "Atmospheric Radiation," Oxford University Press (1964).
18. J. Humlicek, "An Efficient Method for Evaluation of the Complex Probability Function: The Voigt Function and its Derivatives," J. Quant. Spect. Rad. Transfer, 21, 309 (1978).

This problem was avoided by defining a single layer for the primary solar path. The single layer approximation, which is only used by the MODTRAN subroutines, requires the calculation of Curtis Godson averaged pressures and temperatures in SSCEO. Significant modifications were required for TRANS. 200 lines of code have been added to this subroutine, but its basic logic remains unaltered. When JBMOD is set equal to one, TRANS

- sets frequency step size to 1 cm^{-1} ,
- bypasses C1DTA, C2DTA, and C3DTA and calls the MODTRAN subroutines,
- interpolates transmittances calculated in 5 cm^{-1} steps for species other than H_2O , O_3 , and O_2 , and
- employs a discretized triangular slit function with FWHM set to $\text{INT}(\text{DV})$ to automatically degrade the 1 cm^{-1} bin results.

In Subsections 5.1.1 and 5.1.3, the calls to MODTRAN subroutines were discussed. Note that the discretized triangular slit function when DV is set to 1 cm^{-1} is a 1 cm^{-1} rectangular slit function, as shown in Figure 3.

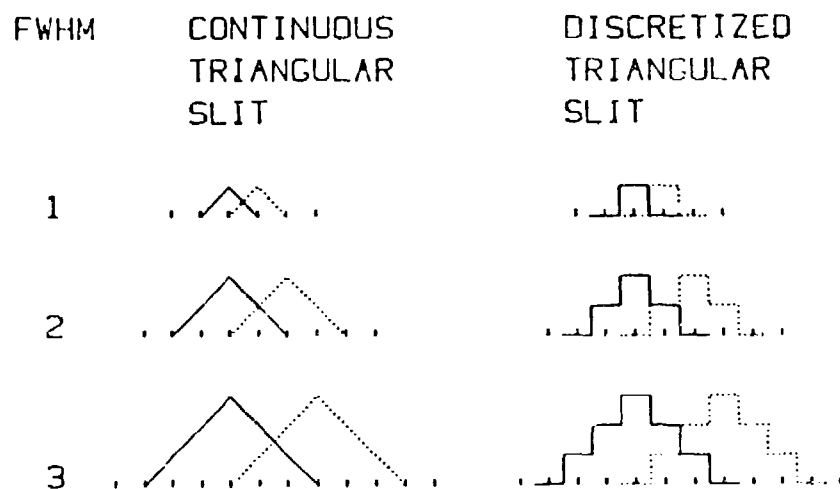


Figure 3. Comparison of Continuous and Discretized Triangular Slit Functions. FASCOD2 Uses the Weighting from the Continuous Function, but MODTRAN Uses the Discretized Approximation.

6.0 VALIDATION

Validation of the band model parameters on the data tape has been completed. However, only a limited amount of testing of MODTRAN's transmittance formulation has been performed thus far. All validation of the code will be by comparison to FASCOD2 results since it is the infinite resolution line by line calculations of FASCOD2 which MODTRAN is attempting to approximate.

6.1 Band Model Parameters

The new band model parameters were validated against the moderate resolution LOWTRAN 5(10,11) values. The 1 cm^{-1} square slit band model parameters can be degraded to $J \text{ cm}^{-1}$ square slit band model parameters (J odd) using the equations

$$(S/d)_{n,i}^{(J)} = \frac{1}{J} \sum_j (S/d)_{n,j}^{(1)} \quad (31)$$

$$(1/d)_{n,i}^{(J)} = J [(S/d)_{n,i}^{(J)}]^2 / \sum_j [(S/d)_{n,j}^{(1)}]^2 / (1/d)_{n,j}^{(1)} \quad (32)$$

$$(\gamma_c)_i^{(J)} = \frac{1}{J (S/d)_n} \sum_j (S/d)_{n,j}^{(1)} (\gamma_c)_j^{(1)} \quad (33)$$

$$M_i^{(J)} = \frac{1}{J (S/d)_n} \sum_j (S/d)_{n,j}^{(1)} M_j^{(1)} \quad (34)$$

$$c_{n,i}^{(J)} \approx c_{n,iJ}^{(1)} - \frac{1}{\pi \Delta \nu^{(1)}} \sum_{j \neq iJ} \frac{(S/d)_{n,j}^{(1)} \gamma_c(T_n P_0)_j^{(1)}}{(j - iJ)^2 + 1/4} \quad (35)$$

where j runs from $iJ - (J-1)/2$ to $iJ + (J-1)/2$. The labels i and j here denote bin indices and the superscripts (1) and (J) refer to the 1 cm^{-1} and $J \text{ cm}^{-1}$ band model parameters, respectively. (Note that the line tail absorption

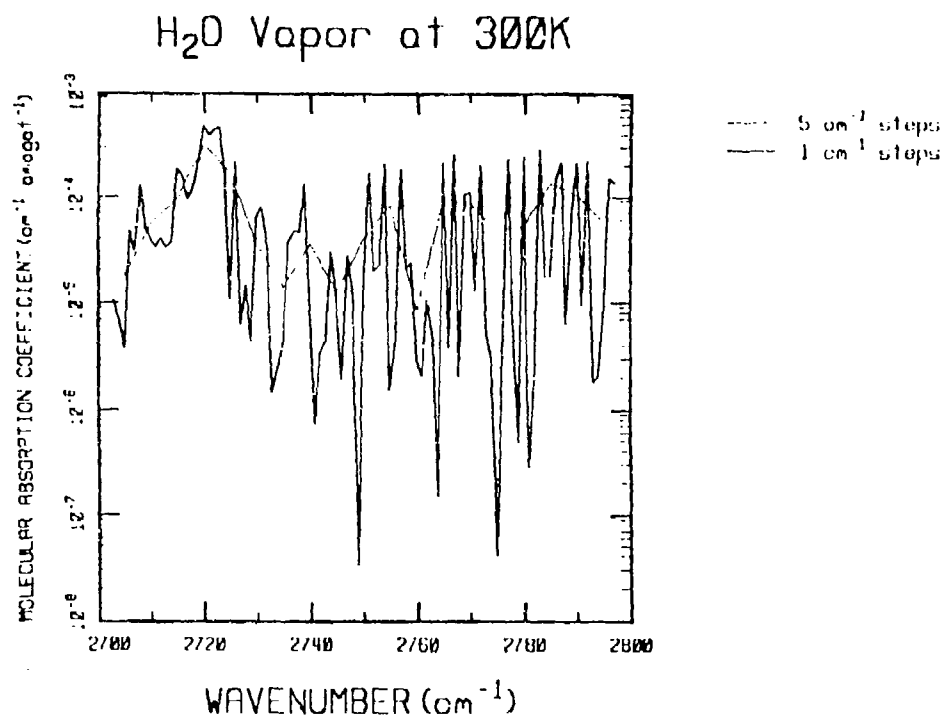


Figure 4. Comparison of Band Model LOWTRAN 5 (Dotted Curve) and Band Model LOWTRAN 6 (Solid Curve) Molecular Absorption Coefficients for Water Vapor at 300 K.

coefficient formula is approximate; an exact expression for its spectral degradation is not derivable.) In Figure 4, the spectral structure of the absorption coefficients is compared. Using these formulas, the 1 cm⁻¹ band model parameters were degraded to 5 cm⁻¹ and then compared to the band model parameters used in the moderate resolution option to LOWTRAN 5. Degradation of the new parameters to 5 cm⁻¹ yields complete agreement.

6.2 Comparison with FASCOD2

In Figure 5, MODTRAN and FASCOD2 transmittance curves are compared for a low altitude slant path through the US Standard Atmosphere in the spectral region 2160–2260 cm⁻¹. The curves were generated with a 1 cm⁻¹ rectangular slit (non overlapping for MODTRAN and overlapping for FASCOD2).

5 - 10 KM AT 15° -- US Std Atm

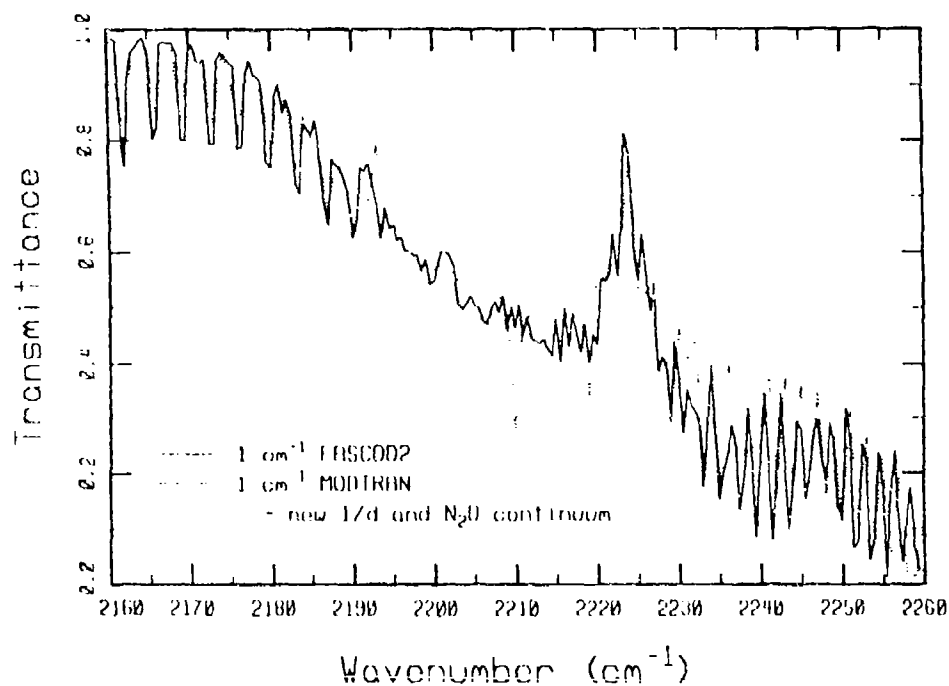


Figure 5. Comparison of a FASCOD2 and a MODTRAN Calculation. N_2O and CO_2 are the Primary Absorbers.

The absorption in this region is primarily due to a N_2O band centered around 2224 cm^{-1} and the P branch of the $4.3 \mu\text{m}$ CO_2 band. Although the agreement is very good, discrepancies do exist. The dip at 2210 cm^{-1} stands out. The N_2O lines in this region are spaced about 0.8 to 0.9 cm^{-1} apart, and therefore most 1 cm^{-1} bins contain just one line. The bin at 2210 cm^{-1} is an exception containing two lines, resulting in the dip. Similar analysis can be applied to other discrepancies and implies that better agreement results with some minimal degradation of the spectral resolution.

Since the band model parameters were generated down to 0 cm^{-1} , MODTRAN can be used to perform molecular absorption calculations in the microwave. Results for a 0.1 km sea level path through the US Standard Atmosphere are compared to FASCOD2 in Figure 6. The comparison is good, but problems are

evident. A series of lines at 7, 11, 13, and 15 cm^{-1} are missing in the MODTRAN calculation. Further investigation is necessary to determine the origin of these discrepancies.

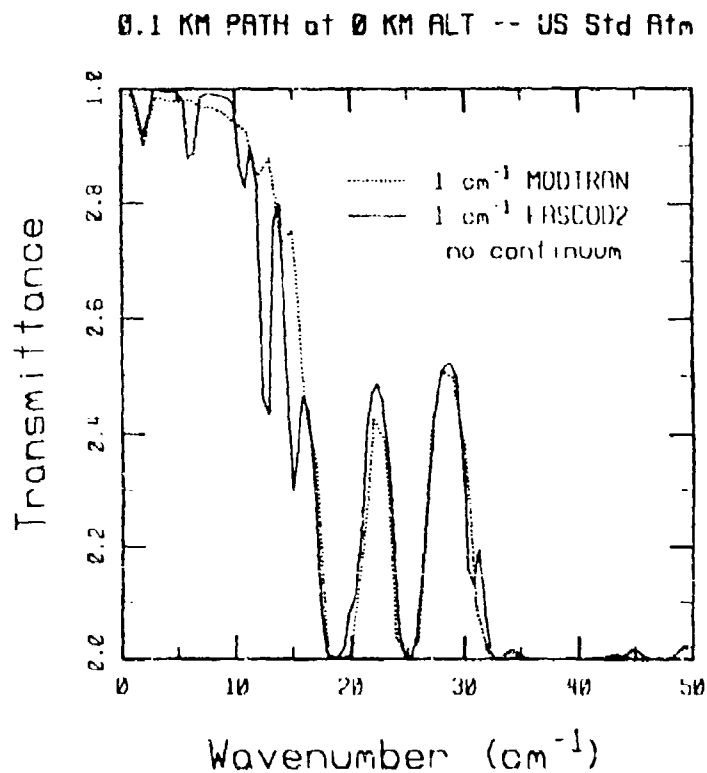


Figure 6. Comparison of a FASCOD2 and a MODTRAN Calculation in the Microwave.

7.0 CONCLUSIONS AND FUTURE WORK

A radiative transfer model applicable to upper altitudes has been developed for LOWTRAN 6. This moderate spectral resolution model has been coded and integrated into LOWTRAN 6. Testing has begun on the new code, referred to as MODTRAN, and a preliminary version has been delivered to the Air Force Geophysics Laboratory.

In the following year, most of our effort will concentrate on validation and optimization of the code. For the frequency range from 0 to $17,900\text{ cm}^{-1}$, MODTRAN and FASCOD2 calculations will be compared for low and high altitude paths. Significant discrepancies will be identified and corrected. After validation is completed, the MODTRAN code will be made more efficient. Methods which may be fruitful for optimizing the code include

- defining cut off values for absorption coefficients,
- combining band model parameters of absorbing species before determining transmittance rather than determining transmittance of each species separately,
- developing a more efficient routine for integrating the Voigt line shape, and/or
- allowing for the spectral resolution of the band model parameters to be degraded internally.

To the extent time permits, each of these approaches will be investigated.

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APPENDIX: DERIVATION OF THE BAND MODEL PARAMETERS

In MODTRAN, the molecular transmittance, τ , from lines originating within a spectral bin, $\Delta\nu$, is determined from an expression of the form

$$\tau = \left(\frac{2}{\Delta\nu} \int_0^{\Delta\nu/2} e^{-Sb(\nu)} d\nu \right)^n \quad (\text{A } 1)$$

where $b(\nu)$ is a line shape function, u is the absorber amount, and S and n are functions of the absorption coefficient (S/d) and line density ($1/d$) band model parameters

$$S = \frac{(S/d)}{(1/d)} \quad (\text{A } 2)$$

$$n = (1/d) \Delta\nu. \quad (\text{A } 3)$$

Eq. (A 1) results from Eqs. (11) and (14a).

A standard method for determining band model parameters was laid out by Goody^(A-1). The weak and strong line limits of a two parameter transmittance expression are determined. These results are equated to the weak and strong line limits of the Ladenburg-Reiche function, and the resulting equations are solved for the unknown parameters. When Goody applied his approach to two trial transmittance formulas, both gave expressions for the band model parameters of the form

$$(S/d) = \frac{1}{\Delta\nu} \sum_{i=1}^N S_i \quad (\text{A } 4)$$

A 1. R. M. Goody, "Atmospheric Radiation," Oxford University Press (1964).

$$(1/d) \approx \frac{1}{\Delta\nu} \left(\sum_{i=1}^N \sqrt{S_i} \right)^2 / \sum_{i=1}^N S_i \quad (A-5)$$

Here, N is the number of lines and S_i is the integrated line strength of line i (the line spacing formula assumes all N lines have the same half width).

It is important to note that Goody's approach is inappropriate for the transmittance expression in MODTRAN. Eq. (A-1) models the transmittance through a set of lines whose centers fall within a given finite spectral bin. The Ladenburg-Reiche function, on the other hand, models the total absorption due to those lines - not just their contribution within a finite spectral bin.

Instead of equating the weak and strong line limit of Eq. (A 1) to the Ladenburg Reiche function, we equate the weak and strong line limit of Eq. (A-1) to Plass' expression^(A 2) for the transmission due to lines whose centers are randomly distributed in a given spectral interval,

$$\left\{ \frac{2}{\Delta\nu} \int_0^{\Delta\nu/2} \exp[-\text{Sub}(\nu)] d\nu \right\}^N \approx \prod_i \left\{ \frac{2}{\Delta\nu} \int_0^{\Delta\nu/2} \exp[-S_i \text{ub}(\nu)] d\nu \right\} \quad (A-6)$$

Here, all N lines are assumed to have the same half width, but the line shape function is arbitrary.

If B_j is defined by the equation

$$B_j \equiv \frac{2}{\Delta\nu} \int_0^{\Delta\nu/2} |b(\nu)|^j d\nu, \quad (A-7)$$

then, in the weak line limit, Eq. (A 6) becomes

A 2. G. N. Plass, "Models for Spectral Band Absorption," J. Opt. Soc. Am., 48, 690 (1958).

$$1 + u (B_1 n S) + u^2 \left[\frac{B_1^2}{2} (n S)^2 + \left(B_2 - \frac{B_1^2}{2}\right) n S^2 \right] + O(u^3) =$$

$$1 + u (B_1 \sum_{i=1}^N S_i) + u^2 \left[\frac{B_1^2}{2} \left(\sum_{i=1}^N S_i\right)^2 + \left(B_2 - \frac{B_1^2}{2}\right) \sum_{i=1}^N S_i^2 \right] + O(u^3). \quad (A 8)$$

The first order equation in u reestablishes Eq. (A 4)

$$n S = \sum_{i=1}^N S_i \quad (A 9)$$

To determine the strong line limit of Eq. (A 6), we assume $b(v)$ to be a non increasing bounded positive function on $[0, \infty)$. Consider a general integral of the form

$$I = \frac{2}{\Delta v} \int_0^{\Delta v/2} e^{-\text{Sub}(v)} dv \quad (A 10)$$

It follows that

$$0 < e^{-\text{Sub}(0)} < 1 < e^{-\text{Sub}(\Delta v/2)} < 1 \quad (A 11)$$

This inequality requires that I falls off exponentially with large u and that the exponent is linear in u . The exponential decay factor, C , is given by the limit as $u \rightarrow \infty$ of the negative logarithm of I divided by u

$$C = - \lim_{u \rightarrow \infty} [\ln(I)/u] \quad (A 12)$$

Applying L'hospital's rule, one obtains

$$C = S \langle b(v) \rangle \quad (A 13)$$

where

$$\langle b(v) \rangle \equiv \lim_{u \rightarrow \infty} \frac{\int_0^{\Delta v/2} b(v) e^{-\text{Sub}(v)} dv}{\int_0^{\Delta v/2} e^{-\text{Sub}(v)} dv}. \quad (\text{A } 14)$$

Note that this limit is independent of the value of S as long as $S > 0$.

Taking the logarithm of both sides of Eq. (A 6), dividing by u , and equating the asymptotic limits, one obtains

$$n S \langle b(v) \rangle = \sum_{i=1}^N S_i \langle b(v) \rangle. \quad (\text{A } 15)$$

Since $\langle b(v) \rangle$ is line independent, the surprising result is that Eq. (A 9), the weak line limit, is also the strong line limit!

To determine n and S , we return to the weak line limit, Eq. (A 8), and consider the equation obtained from the coefficient of the quadratic terms in u . This equation gives

$$n S^2 = \sum_{i=1}^N S_i^2. \quad (\text{A } 16)$$

The resulting expressions for the band model parameters are

$$(S/d) = \frac{1}{\Delta v} \sum_{i=1}^N S_i \quad (\text{A } 4)$$

$$(1/d) = \frac{1}{\Delta v} \left(\sum_{i=1}^N S_i \right)^2 / \sum_{i=1}^N S_i^2 \quad (\text{A } 17)$$

(S/d) has the same form as before, but a smaller value for $(1/d)$ is obtained, because the weaker lines are weighted less in Eq. (A 17) than in Eq. (A 5).

Figures 5 and A-1 compare a 1 cm^{-1} non-overlapping rectangular slit MODTRAN calculation with the new and old band model parameters to a 1 cm^{-1} overlapping rectangular slit FASCOD2 calculation. The results with the new formulation are much improved. Further investigation and validation are planned.

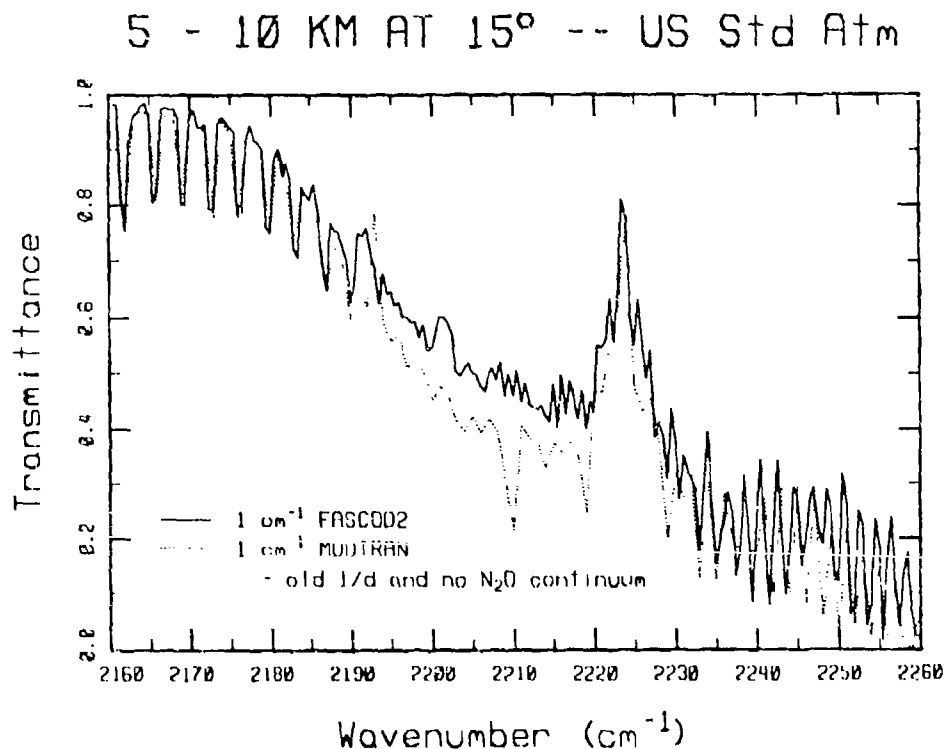


Figure A-1. Comparison of FASCOD2 and MODTRAN Calculations. The MODTRAN Curve was Generated with the Old Band Model Parameters, Eqs. (A-4) & (A-5), and no N_2O Continuum Function.

REFERENCES

- A-1. R. M. Goody, "Atmospheric Radiation," Oxford University Press, 1964.
- A-2. G. N. Plass, "Models for Spectral Band Absorption," J. Opt. Soc. Am., 48, 690 (1958).